

# Surface and corner free energies of the self-dual Potts model

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## Abstract

We consider the bulk, vertical surface, horizontal surface and corner free energies  $f_b, f_s, f'_s, f_c$  of the anisotropic self-dual  $Q$ -state Potts model for  $Q > 4$ .  $f_b$  was calculated in 1973[1]. For  $Q < 4$ ,  $f_s, f'_s$  were calculated in 1989[2]. Here we extend this last calculation to  $Q > 4$  and find agreement with the conjectures made in 2012 by Vernier and Jacobsen (VJ)[3] for the isotropic case. All these four free energies satisfy inversion and rotation relations. Together with some plausible analyticity assumptions, these provide a less rigorous, but much simpler, way of determining  $f_b, f_s, f'_s$ . They also imply that  $f_c$  is independent of the anisotropy, being a function only of  $Q$ , in which respect they resemble the order parameters of the associated six-vertex model. Hence VJ's conjecture for  $f_c$  should apply to the full anisotropic model.

KEY WORDS: Statistical mechanics, lattice models, exactly solved models, surface and corner free energies

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# 1 Introduction

Vernier and Jacobsen[3] considered a number of two-dimensional lattice models in statistical mechanics for which the bulk free energies have been calculated exactly and conjectured their surface and corner free energies. They considered only the rotation-invariant (isotropic) cases of these models, when the surface free energies are the same for the vertical and horizontal surfaces.

For some of these models the surface free energies have been, or can readily be, calculated exactly, and this can be done for the more general non-rotation-invariant cases. For the case of the square-lattice self-dual Potts model, Vernier and Jacobsen commented that it seemed likely that the surface free energy had been calculated. It seems that this has not yet been reported in the literature for the case in which they were interested. That omission is repaired here for the general anisotropic case.

We also present arguments that Vernier and Jacobsen’s[3] conjecture for the corner free energy should apply to the anisotropic case.

Consider the self-dual  $Q$ -state Potts model on the square lattice, which is equivalent to an homogeneous six-vertex model.[4, §12.5] Owczarek and Baxter[2] showed that for this model an extended Bethe ansatz worked for a lattice of  $N$  columns with free (rather than cylindrical) boundary conditions. They wrote down the resulting “Bethe equations” for the eigenvalues of the row-to-row transfer matrix  $T$ . They were interested in the critical case, which occurs when the number of states  $Q$  is not greater than 4, and solved the equations for  $N$  large to obtain the bulk and surface free energies.

Vernier and Jacobsen[3, §3.2.1] instead considered the case  $Q > 4$ , when the model is at a first-order transition point. Here we solve the Bethe equations for this case. We obtain the surface free energies  $f_s$  and  $f'_s$  (as well as the bulk free energy  $f_b$ ) and verify the correctness of Vernier and Jacobsen’s conjectures for the rotation-invariant case.

We also show that the four free energies all satisfy “inversion” and “rotation” relations, and that if we assume certain plausible analyticity properties, then these are sufficient to determine the bulk and surface free energies, and to show that the corner free energy is independent of the anisotropy of the model, depending only on  $Q$ . The results of this method of course agree with those of the more rigorous Bethe ansatz calculations.

The self-dual Potts model contains two free parameters  $Q, K_1$ , or equivalently the  $q, w$  defined by (2.5), (3.1), (3.7), (3.11).<sup>1</sup> Our Bethe ansatz method is not sufficient to calculate the corner free energy  $f_c$ , but the inversion relation method implies that it is independent of  $K_1$  or  $w$ , depending only on  $Q$  or  $q$ . We also comment in section 4 that we have performed direct numerical calculations on finite lattices to obtain the first 10 coefficients in a series expansion in powers of  $q$  as functions of  $s = w^2/q^{1/2}$ . (Each coefficient is a finite Laurent polynomial in  $s$ .) We find agreement (as expected) with Vernier and Jacobsen's,[3, §3.2.1] conjecture for the isotropic case,<sup>2</sup> which is when  $w = q^{1/4}$  and  $s = 1$ .

For the corner free energy  $f_c$ , we also observe that all the 10 coefficients are *independent* of  $s$ , which agrees with the inversion relation result that  $f_c$  is a function only of  $q$ .

For this model, therefore,  $f_c$  resembles the order parameters  $M_0$  and  $P_0$  of the associated six-vertex model,[4, eqn. 8.10.9], in that it depends only on  $Q$  or  $q$ .

We have found corresponding behaviour for the square-lattice Ising model.[7] For both models, this means that the corner free energy is a function only of the order parameter. Possibly this property applies more generally.

## 2 The square-lattice Potts model

We consider the  $Q$ -state Potts model on a square lattice  $\mathcal{L}$  of  $M$  rows and  $N$  columns, as shown in Fig. 1. On each site  $i$  there is a "spin"  $\sigma_i$  that takes the values  $1, 2, \dots, Q$ . Spins at horizontally adjacent sites  $i, j$  interact with dimensionless energy  $-K_1\delta(\sigma_i, \sigma_j)$ , and those on vertically adjacent sites with energy  $-K_2\delta(\sigma_k, \sigma_m)$ .

The partition function is

$$Z_P = \sum_{\sigma} \exp \left[ K_1 \sum \delta(\sigma_i, \sigma_j) + K_2 \sum \delta(\sigma_k, \sigma_m) \right] , \quad (2.1)$$

where the first inner sum is over all horizontal edges  $(i, j)$  and the second over all vertical edges  $(k, m)$ . The outer sum is over all  $Q^{MN}$  values of all the spins.

We expect that when  $M, N$  are large,

$$\log Z_P = -MNf_b - Mf_s - Nf'_s - f_c + O(e^{-\delta M}, e^{-\delta' N}) , \quad (2.2)$$

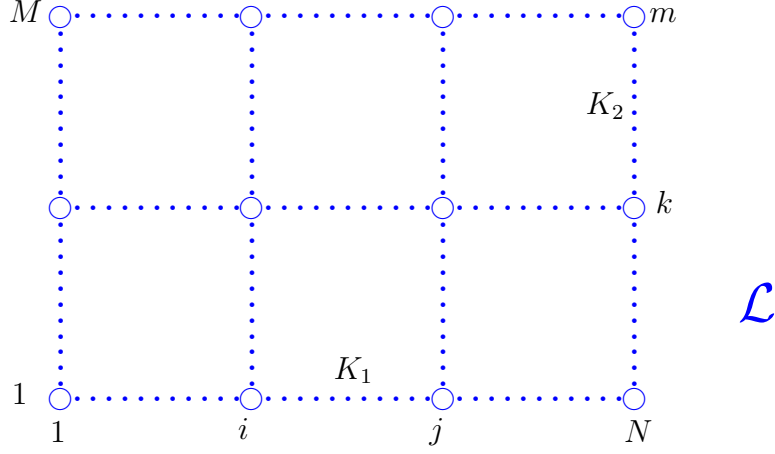
where  $f_b, f_s, f'_s, f_c$  are the dimensionless bulk, vertical surface, horizontal surface and corner free energies, and  $\delta, \delta'$  are positive numbers.

We show in [4, §12.5] that this model is equivalent to a six-vertex model on the lattice  $\mathcal{L}'$  of Fig. 2, i.e the lattice of solid lines and circles therein. On this lattice we place an arrow on each edge subject to the rule that at each site or vertex there must be as many arrows pointing in as there are pointing out.

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<sup>1</sup>From these equations,  $Q = q + 2 + q^{-1}$ .

<sup>2</sup> $q$  herein is  $q_{VJ}^2$ , where  $q_{VJ}$  is the  $q$  of Vernier and Jacobsen, and all the free energies are negated.



**Figure 1:** The square lattice  $\mathcal{L}$  (of 3 rows and 4 columns), indicating the horizontal and vertical interaction coefficients  $K_1, K_2$ .

There are six such configurations of arrows at an internal vertex, as shown in Fig. 3.

The lattice  $\mathcal{L}'$  has  $2M+1$  rows, even-numbered rows having  $N+1$  vertices, and odd-numbered ones having  $N$  vertices. Between two successive rows there are  $2N$  diagonal edges, on which one places arrows. Each of the  $M$  even-numbered rows has  $N-1$  internal vertices, with weights

$$\omega_1, \dots, \omega_6 = 1, x_1, x_1, 1 + x_1 e^\lambda, 1 + x_1 e^{-\lambda}, \quad (2.3)$$

and each of the  $M-1$  odd-numbered rows  $3, 5, \dots, 2M-1$  has  $N$  internal vertices with weights

$$\omega_1, \dots, \omega_6 = x_2, x_2, 1, 1, x_2 + e^\lambda, x_2 + e^{-\lambda}, \quad (2.4)$$

where

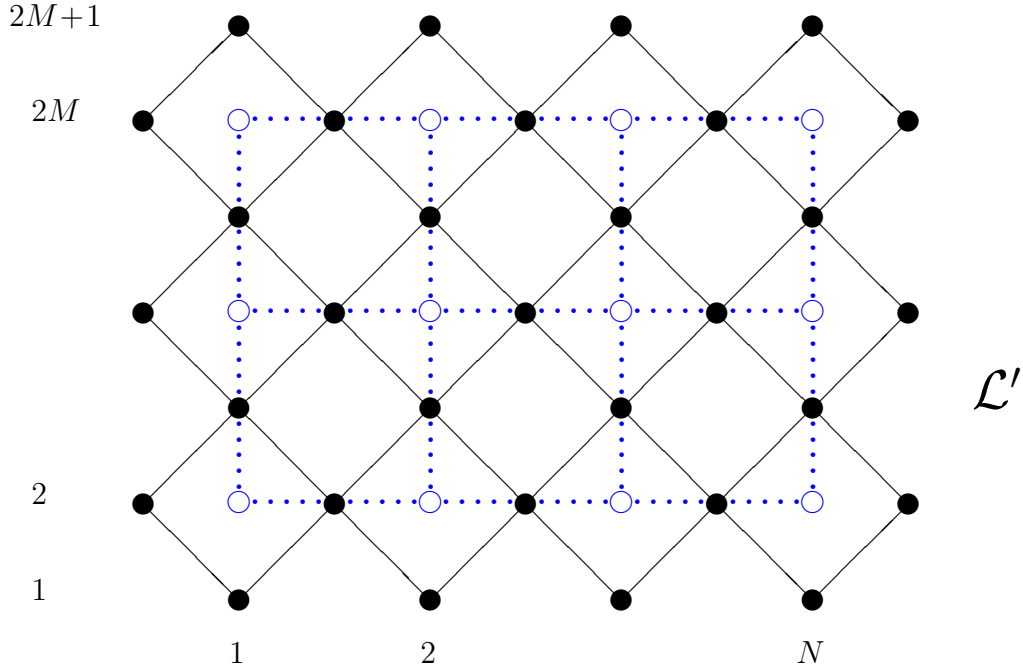
$$Q^{1/2} = 2 \cosh \lambda, \quad x_1 = (e^{K_1} - 1)/Q^{1/2}, \quad x_2 = (e^{K_2} - 1)/Q^{1/2}. \quad (2.5)$$

The vertices on the boundaries of  $\mathcal{L}'$  only have two edges joining them and must have one arrow in and one arrow out. The weights of the possible configurations are indicated in Fig. 4.

The partition function of this six-vertex model is

$$Z_{6V} = \sum_C \prod_i w_i, \quad (2.6)$$

where the sum is over all allowed configurations  $C$  of arrows on the edges of  $\mathcal{L}'$  and for each configuration the product is over all vertices  $i$  of the corresponding weights  $w_i$  (including the boundary vertices).



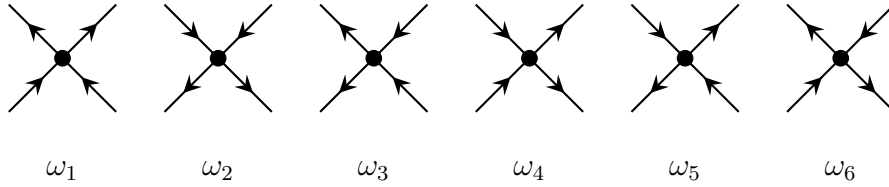
**Figure 2:** The square lattice  $\mathcal{L}$  of dotted lines and circles, and its medial lattice  $\mathcal{L}'$  of full circles and lines .

If  $\mathcal{L}'$  were wound on a torus (which is *not* the case considered in this paper), we could interchange the two types of rows without affecting the partition function. This is equivalent to replacing  $x_1, x_2$  by  $x_1^* = 1/x_2, x_2^* = 1/x_1$  and multiplying  $Z_P$  by  $(x_1/x_2)^{MN}$ , and to replacing  $K_1, K_2$  by their “duals”  $K_1^*, K_2^*$ , where

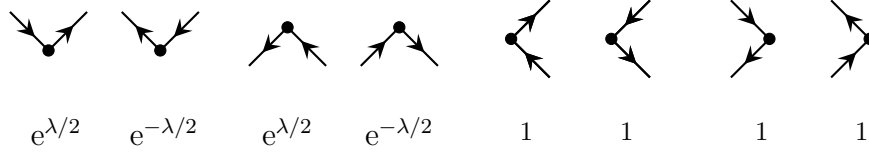
$$\exp(K_1^*) = \frac{e^{K_2} + Q - 1}{e^{K_2} - 1} \quad , \quad \exp(K_2^*) = \frac{e^{K_1} + Q - 1}{e^{K_1} - 1} \quad . \quad (2.7)$$

The partition function  $Z$  of the Potts model, as defined in (2.1), is related exactly to  $Z_{6V}$  by

$$Z_P = Q^{MN/2} Z_{6V} \quad (2.8)$$



**Figure 3:** The six vertices, with weights  $\omega_1, \dots, \omega_6$ .



**Figure 4:** The boundary weights.

Let  $T_1$  be the row-to-row transfer matrix for an odd row of  $\mathcal{L}'$ , and  $T_2$  the transfer matrix for an even row. Then

$$Z_{6V} = \langle 0 | T_1 T_2 T_1 \cdots T_2 T_1 | 0 \rangle , \quad (2.9)$$

where there are  $M$  factors  $T_1$  in the matrix product, and  $M - 1$  factors  $T_2$ , and  $\langle 0 |$ ,  $| 0 \rangle$  are vectors that account for the bottom and top boundaries of  $\mathcal{L}'$ . Let  $\Lambda^2$  be a typical eigenvalue of  $T_1 T_2$ , given by the equations

$$\Lambda f = T_1 g , \quad \Lambda g = T_2 f , \quad (2.10)$$

$f, g$  being the associated eigenvectors.

The right-hand side of (2.9) can be written as a sum over terms, each proportional to  $\Lambda^{2M}$ . In the limit of  $M$  large, this will be given by

$$Z_{6V} = C \Lambda_{\max}^{2M} [1 + O(e^{-\gamma M})] , \quad (2.11)$$

where  $\Lambda_{\max}$  is the maximum eigenvalue and  $Re(\gamma) > 0$ . In the limit of  $M$  large it follows that

$$\lim_{M \rightarrow \infty} (\log Z_{6V}) / M = \log \Lambda_{\max}^2 . \quad (2.12)$$

### 3 The self-dual Potts model, with $x_1 x_2 = 1$

For general  $x_1, x_2$  the Bethe ansatz does not work for this inhomogeneous model. However, if  $x_2 = 1/x_1$ , we can define

$$x_1 = x , \quad x_2 = 1/x , \quad (3.1)$$

and then the weights for the internal vertices on odd and even rows, given in (2.3) and (2.4) satisfy

$$(\omega_1, \dots, \omega_6)_{\text{odd}} = x^{-1} (\omega_1, \dots, \omega_6)_{\text{even}} \quad (3.2)$$

so

$$Z_{6V} = x^{-N(M-1)} Z_{\text{hom}} , \quad (3.3)$$

where  $Z_{\text{hom}}$  is the partition function of a six-vertex model defined in the same way as previously, but with all internal weights given by (2.3), so it is homogeneous (but not rotation-invariant). We note from (2.2), (2.8), (2.12), (3.3) that

$$-N f_b - f_s = (N/2) \log Q - N \log x + \log \Lambda_0^2 \quad (3.4)$$

to within terms of order  $e^{-\delta'N}$ ,  $\Lambda_0$  being the maximum eigenvalue of the transfer matrix of the homogeneous model.

The corresponding Potts model is self-dual, with

$$K_1^* = K_2 \quad , \quad K_2^* = K_1 \quad . \quad (3.5)$$

One must still distinguish between  $T_1$  and  $T_2$  because the boundary conditions are different for the two type of row. However, Owczarek and Baxter[2] were able to solve (2.10) by extending the Bethe ansatz to free boundary conditions (for every wave number  $k$  there is a reflected wave number  $-k$ ).

The number  $n$  of down arrows between two successive rows of  $\mathcal{L}'$  is conserved in this model. Owczarek and Baxter[2] solved (2.10) for arbitrary  $n$ , but the top and bottom boundary conditions ensure that  $n = N$  (there are as many down arrows as up ones), and we shall only consider this case.

Our notation here is not quite consistent with [2], one significant difference being that  $N$  in that paper is  $2N$  here.

To make the notation for the weights consistent, associate an extra weight  $t$  with the top of every down-pointing NW -SE arrow, and a weight  $1/t$  with the bottom of every such arrow. Then the first four weights  $\omega_1, \dots, \omega_6$  in Fig. (3) are unchanged, while  $\omega_5, \omega_6$  become  $t^{-1}\omega_5, t\omega_6$ . The eight boundary weights in Fig. (4) are multiplied by  $t^{-1}, 1, 1, t, 1, t, t^{-1}, 1$ , respectively. Taking  $t$  to be as in [2], and  $\lambda$  herein to be given by

$$e^{\lambda/2} = t \quad , \quad (3.6)$$

we obtain the weights of (2.64) – (2.67) of [2],  $q$  therein being the  $Q$  of this paper.

These additional edge weights cancel out of the partition function and of the eigenvalue  $\Lambda$ .

The parameter  $\mu$  of [2] is given by  $\mu = i\lambda$  and we replace  $v$  therein by  $v = \mu - 2iu$  so

$$x = \frac{\sinh(\lambda - 2u)}{\sinh 2u} \quad . \quad (3.7)$$

Then equations (2.86), (2.87), (2.74) of [2] become (replacing  $n, N$  therein by  $N, 2N$ )

$$\Lambda^2 = \prod_{j=1}^N \frac{\sinh(\lambda - u - \alpha_j) \sinh(\lambda - u + \alpha_j)}{\sinh(u - \alpha_j) \sinh(u + \alpha_j)} \quad , \quad (3.8)$$

where  $\alpha_1, \dots, \alpha_N$  are given by the  $N$  “Bethe equations”

$$\left[ \frac{\sinh(u + \alpha_j) \sinh(\lambda - u + \alpha_j)}{\sinh(u - \alpha_j) \sinh(\lambda - u - \alpha_j)} \right]^{2N} = \prod_{m=1, m \neq j}^N \frac{\sinh(\lambda + \alpha_j - \alpha_m) \sinh(\lambda + \alpha_j + \alpha_m)}{\sinh(\lambda + \alpha_m - \alpha_j) \sinh(\lambda - \alpha_j - \alpha_m)} \quad (3.9)$$

for  $j = 1, \dots, N$ .

(3.9) has many solutions, corresponding to the various eigenvalues. We are only concerned with the maximum eigenvalue.

### 3.1 Solution of the Bethe equations

If the number of states  $Q$  is less than four, then  $\lambda$  is pure imaginary and the large- $N$  solution of (3.9) is given in [2].

If  $Q > 4$ , then  $\lambda$  is real and positive. For the ferromagnetic Potts model, from (2.5)  $x$  is real and positive so

$$0 < u < \lambda/2 . \quad (3.10)$$

Here we obtain the large- $N$  behaviour of the maximum eigenvalue  $\Lambda_{\max}$  for this case, using a method similar to that given in Appendix D of [8] for the eight-vertex model.

First write (3.8), (3.9) in terms of polynomials in the variables

$$q = e^{-2\lambda} , \quad w = e^{-2u} , \quad z_j = e^{-2\alpha_j} \quad (3.11)$$

as

$$\Lambda^2 = (w^{2N}/q^N) \prod_{j=1}^N \frac{(1 - q/wz_j)(1 - qz_j/w)}{(1 - w/z_j)(1 - wz_j)} , \quad (3.12)$$

$$z_j^{-4N} \left[ \frac{(1 - wz_j)(1 - qz_j/w)}{(1 - w/z_j)(1 - q/wz_j)} \right]^{2N} = z_j^{2-2N} \frac{(1 - q/z_j^2)}{(1 - qz_j^2)} \prod_{m=1}^N \frac{(1 - qz_j z_m)(1 - qz_j/z_m)}{(1 - qz_m/z_j)(1 - q/z_j z_m)} , \quad j = 1, \dots, N . \quad (3.13)$$

Consider the limit when  $q, w \rightarrow \infty$ . From (3.10), the largest of  $q, w, q/w$  is  $w$ , so if we take  $w \rightarrow 0$ , then it is also true that  $q, q/w \rightarrow 0$ . Suppose that  $z_1, \dots, z_N$  remain of order one. Then (3.13) becomes

$$z_j^{2N+2} = 1 , \quad j = 1, \dots, N . \quad (3.14)$$

This has  $2N + 2$  solutions for  $z_j$ .

The Bethe ansatz used in [2] is a sum over all permutations and inversions of  $z_1, \dots, z_N$ . If any  $z_j$  is equal to its inverse, or if any two are equal to one another, or to their inverses, then the Bethe ansatz gives a zero eigenvector, which must be rejected. Replacing any  $z_j$  (or  $z_m$ ) in (3.12), (3.13) by its inverse does not change the equations.

We therefore reject the solutions  $z_j = \pm 1$  of (3.14), and group the remaining  $2N$  solutions into  $N$  distinct pairs  $z_j, 1/z_j$ . Equivalently, we require  $z_1, \dots, z_N$  to be distinct and to lie in the upper half of the complex plane.

Then there is a unique solution of (3.14) for the  $z_1, \dots, z_N$ , and the corresponding eigenvalue in this limit is

$$\Lambda^2 = w^{2N}/q^N . \quad (3.15)$$

This is indeed then the maximum eigenvalue  $\Lambda_0$ , corresponding to all the left-hand arrows in  $\mathcal{L}'$  being down, and the arrows then alternating in direction



from left to right. The  $N$  vertices in odd rows are in configuration 5, those in even rows in configuration 6.

Now define the functions

$$r(z) = (1 - wz)^{2N} (1 - qz/w)^{2N} (1 - qz^2) , \quad (3.16)$$

$$R(z) = \prod_{m=1}^N (1 - z/z_m)(1 - z z_m) , \quad (3.17)$$

$$S(z) = \frac{z^{2N+2} r(1/z)}{R(q/z)} - \frac{r(z)}{R(qz)} . \quad (3.18)$$

Then (3.12), (3.13) can be written simply as

$$\Lambda^2 = \frac{w^{2N} R(q/w)}{q^N R(w)} , \quad (3.19)$$

$$S(z_j) = 0 , \quad j = 1, \dots, N . \quad (3.20)$$

$S(z)$  therefore has zeros when  $z = z_m$  or  $z = 1/z_m$ . It also has zeros at  $z = 1$  and  $z = -1$ . It is of course a rational function, but if we take  $z, z_m$  to be of order unity and expand in powers of  $q, w$  and  $q/w$ , then to order  $w^{2N}$ ,  $S(z)$  remains a polynomial of degree  $2N + 2$ . To this order therefore, we can set

$$S(z) = (z^2 - 1)R(z) . \quad (3.21)$$

Further, the terms proportional to  $z^{2N+2}, z^{2N+1}, z^{2N}, \dots, z^{N+2}$  come solely from the first term on the RHS of (3.18), while the terms proportional to  $1, z, z^2, \dots, z^N$  come from the second term. Using the second feature, it follows that for  $|z| < 1$ ,

$$\frac{r(z)}{R(qz)} = (1 - z^2)R(z) . \quad (3.22)$$

More accurately, if  $|z| < e^{-\delta}$ , then (3.22) is true to relative order  $e^{-N\delta}$ .

Since this is true for  $|z| < 1$ , it is more strongly true for  $|z| < q$ , so we can replace  $z$  by  $qz$  to obtain

$$\frac{r(qz)}{R(q^2z)} = (1 - q^2z^2)R(qz) . \quad (3.23)$$

Proceeding in this way, noting that  $R(z) \rightarrow 1$  as  $z \rightarrow 0$ , we can solve the equations (3.22), (3.23),  $\dots$ , for  $R(z)$  to obtain

$$R(z) = \prod_{k=0}^{\infty} \frac{(1 - q^{4k+2}z^2) r(q^{2k}z)}{(1 - q^{4k}z^2) r(q^{2k+1}z)} , \quad |z| < 1 , \quad (3.24)$$

i.e.

$$R(z) = \prod_{k=0}^{\infty} \frac{(1 - q^{4k+1}z^2)(1 - q^{4k+2}z^2)}{(1 - q^{4k}z^2)(1 - q^{4k+3}z^2)} \left[ \frac{(1 - q^{2k}wz)(1 - q^{2k+1}z/w)}{(1 - q^{2k+1}wz)(1 - q^{2k+2}z/w)} \right]^{2N}$$

or

$$\log R(z) = \sum_{n=1}^{\infty} \frac{(1 - q^n)z^{2n}}{n(1 + q^{2n})} - 2N \sum_{n=1}^{\infty} \frac{(w^n + q^n/w^n)z^n}{n(1 + q^n)} . \quad (3.25)$$

### 3.1.1 The free energies

Substituting (3.25) into (3.19), we get, to within additional terms that vanish exponentially fast as  $N$  becomes large,

$$\log \Lambda_0^2 = N \left[ \log \frac{w^2}{q} + 2 \sum_{n=1}^{\infty} \frac{(w^{2n} - q^{2n} w^{-2n})}{n(1 + q^n)} \right] - \sum_{n=1}^{\infty} \frac{(1 - q^n)(w^{2n} - q^{2n} w^{-2n})}{n(1 + q^{2n})}$$

so from (3.4), the bulk and surface free energies of the original Potts model of (2.1) and (2.2) are

$$f_b = -\frac{1}{2} \log Q + \log x - \log \frac{w^2}{q} - 2 \sum_{n=1}^{\infty} \frac{(w^{2n} - q^{2n} w^{-2n})}{n(1 + q^n)} , \quad (3.26)$$

$$f_s = \sum_{n=1}^{\infty} \frac{(1 - q^n)(w^{2n} - q^{2n} w^{-2n})}{n(1 + q^{2n})} . \quad (3.27)$$

From (2.5), (3.7)

$$Q = q + 2 + q^{-1} , \quad x = \frac{w^2(1 - q/w^2)}{q^{1/2}(1 - w^2)} ,$$

so

$$f_b = \log \left( \frac{q}{1 + q} \right) - \sum_{n=1}^{\infty} \frac{(1 - q^n)(w^{2n} + q^n/w^{2n})}{n(1 + q^n)} \quad (3.28)$$

which is the same result as that of eqns. (12.5.5) and (12.5.6c) of [4],  $q, \psi, \beta$  therein being the  $Q, f_b, \lambda - 2u$  of this paper. We can also write (3.28), (3.27) as

$$f_b = -K_1 - K_2 - \log(1 + q) + \sum_{n=1}^{\infty} \frac{q^n(1 - q^n)(w^{2n} + q^n/w^{2n})}{n(1 + q^n)} , \quad (3.29)$$

$$f_s = \log \left( \frac{1 - q^2/w^2}{1 - w^2} \right) - \sum_{n=1}^{\infty} \frac{q^n(1 + q^n)(w^{2n} - q^{2n} w^{-2n})}{n(1 + q^{2n})} . \quad (3.30)$$

Rotating the model through  $90^\circ$  is equivalent to inverting  $x$ , i.e. of replacing  $u$  by  $\lambda/2 - u$ , and of replacing  $w$  by  $q^{1/2}/w$ . We see that this does indeed leave the RHS of (3.28) unchanged. Also, making this rotation we obtain from (3.27) the result

$$f'_s = \sum_{n=1}^{\infty} \frac{q^n(1 - q^n)(w^{-2n} - w^{2n})}{n(1 + q^{2n})} \quad (3.31)$$

for the horizontal surface free energy.

## 4 The isotropic case conjectures of Vernier and Jacobsen

### 4.1 Bulk and surface free energies

Vernier and Jacobsen[3] negated the free energies, here we revert to the conventional signs, as given in (2.2). As we noted earlier, if  $q_{VJ}$  is their  $q$ , then our  $q = q_{VJ}^2$ . For the rotationally invariant case, when  $w = q^{1/4}$ , they obtained

$$e^{-f_b} = \frac{(1+q)}{q(1-q^{1/2})^2} \prod_{k=1}^{\infty} \left( \frac{1-q^{2k-1/2}}{1-q^{2k+1/2}} \right)^4. \quad (4.1)$$

Taking logarithms, this gives

$$f_b = \log \left( \frac{q}{1+q} \right) - 2 \sum_{n=1}^{\infty} \frac{q^{n/2} (1-q^n)}{n(1+q^n)}. \quad (4.2)$$

They observed that this does indeed agree with the known result (3.28) above.

They also conjectured that

$$e^{-f_s} = (1-q^{1/2}) \prod_{k=1}^{\infty} \left( \frac{1-q^{4k-1/2}}{1-q^{4k-5/2}} \right)^2, \quad (4.3)$$

i.e.

$$f_s = \sum_{n=1}^{\infty} \frac{q^{n/2} (1-q^n)^2}{n(1+q^{2n})}. \quad (4.4)$$

Again, this agrees with the our result (3.27) when  $w = q^{1/4}$ .

### 4.2 The corner free energy

Vernier and Jacobsen[3] also conjectured from their series expansions that the corner free energy is given by

$$e^{-f_c} = \prod_{k=1}^{\infty} \frac{1}{(1-q^{4k-3})(1-q^{4k-2})^4(1-q^{4k-1})}, \quad (4.5)$$

i.e.

$$f_c = - \sum_{n=1}^{\infty} \frac{q^n + 4q^{2n} + q^{3n}}{n(1-q^{4n})}. \quad (4.6)$$

### 4.3 Our series expansions

We have also used series expansions to test Vernier and Jacobsen conjectures. We put the six-vertex model into interaction-round-a-face (IRF) form[4, §10.3] and calculated the finite-size partition function by dividing it into four corners, as in the corner transfer matrix method[4, Fig. 13.2], and building up the lattice by going round the centre spin. We took

$$w = q^{1/4} s^{1/2} \quad (4.7)$$

and expanded  $f_b, f_s, f'_s, f_c$  in powers of  $q$  for given  $s$ . The coefficients of the expansion are Laurent polynomials in  $s$ , and in the isotropic (rotation-invariant) case  $s$  is equal to one.

This was reasonably efficient, but we were only able to get to order  $q^9$ , whereas Vernier and Jacobsen[3, §3.2] went to order  $q^{31/2}$ . We of course agreed with them for  $s = 1$ .

For general  $s$ , we found, to the order to which we went, that  $f_c$  was *independent* of  $s$  (i.e. all the coefficients were constants), suggesting that this is true to all orders and  $f_c$  is exactly independent of  $s$  or  $w$ , being a function only of  $q$ . This agrees with our result for  $f_c$  of the next section.

## 5 Inversion relations

From (2.5) and (3.1),

$$e^{K_1} = 1 + Q^{1/2}x \quad , \quad e^{K_2} = 1 + Q^{1/2}/x \quad , \quad (5.1)$$

so from (3.7),

$$\begin{aligned} e^{K_1} &= \frac{\sinh(2\lambda - 2u)}{\sinh 2u} = \frac{w^2}{q} \frac{1 - q^2/w^2}{1 - w^2} \quad , \\ e^{K_2} &= \frac{\sinh(\lambda + 2u)}{\sinh(\lambda - 2u)} = \frac{1}{w^2} \frac{1 - qw^2}{1 - q/w^2} \quad . \end{aligned} \quad (5.2)$$

We regard these equations as defining  $K_1, K_2$  as functions of the variable  $u$ . Then

$$e^{K_1(u)} e^{K_1(\lambda - u)} = 1 \quad , \quad e^{K_2(\lambda - u)} = \frac{\sinh(3\lambda - 2u)}{\sinh(2u - \lambda)} = 2 - Q - e^{K_2(u)} \quad (5.3)$$

The row-to-row transfer matrix of the Potts model, as formulated in (2.1), is  $\tilde{T}_1 \tilde{T}_2$ , where

$$(\tilde{T}_1)_{\sigma, \sigma'} = \delta(\sigma, \sigma') \prod_{j=1}^{N-1} e^{K_1 \delta(\sigma_j, \sigma_{j+1})} \quad , \quad (\tilde{T}_2)_{\sigma, \sigma'} = \prod_{j=1}^N e^{K_2 \delta(\sigma_j, \sigma'_j)} \quad (5.4)$$

writing  $\sigma = \sigma_1, \dots, \sigma_N$  for all the  $N$  spins in a row, and similarly for the spins  $\sigma' = \sigma'_1, \dots, \sigma'_N$  in the row above. Regarding  $\tilde{T}_1, \tilde{T}_2$  as functions of the variable  $u$ , it follows that

$$\tilde{T}_1(u) \tilde{T}_1(\lambda - u) = \mathbf{1} \quad , \quad \tilde{T}_2(u) \tilde{T}_2(\lambda - u) = \xi(u)^N \mathbf{1} \quad , \quad (5.5)$$

where  $\mathbf{1}$  is the  $Q^N$ -dimensional identity matrix and

$$\xi(u) = e^{K_2(u)} e^{K_2(\lambda - u)} + Q - 1 = - \frac{Q \sinh(2u) \sinh(2\lambda - 2u)}{\sinh(\lambda - 2u)^2} \quad . \quad (5.6)$$

Define the combined transfer matrix

$$V = T_2^{1/2} T_1 T_2^{1/2} \quad (5.7)$$

and let  $|0\rangle$  and  $\langle 0|$  be the  $Q^N$ -dimensional column and row vectors all of whose entries are one. Then from (2.1)

$$Z_P = \langle 0|T_1T_2T_1\cdots T_2T_1|0\rangle = \langle 0|T_2^{-1/2}V^MT_2^{-1/2}|0\rangle . \quad (5.8)$$

Let

$$\Delta = \Delta(u) = e^{K_2} + Q - 1 = \frac{2 \cosh \lambda \sinh(2\lambda - 2u)}{\sinh(\lambda - 2u)} , \quad (5.9)$$

then from (5.4),

$$T_2|0\rangle = \Delta^N|0\rangle , \quad (5.10)$$

so  $|0\rangle$  is an eigenvector of  $T_2$  and

$$T_2^{-1/2}|0\rangle = \Delta^{-N/2}|0\rangle . \quad (5.11)$$

Hence (5.8) can be written

$$Z_P = \Delta^{-N} \langle 0|V^M|0\rangle . \quad (5.12)$$

The  $\Lambda^2$  of (2.10) is also the eigenvalue of  $V$ , so if we neglect only terms that are relatively exponentially small when  $M$  is large, we can write (5.12) as

$$Z_P = \Delta^{-N} \Lambda_{\max}^{2M} \langle \psi|0\rangle^2 , \quad (5.13)$$

where  $\psi$  is the maximal eigenvector of  $V$ :

$$V\psi = \Lambda_{\max}^2 \psi . \quad (5.14)$$

The number of rows  $M$  enters (5.13) only explicitly ( $\Lambda_{\max}$  and  $\psi$  are independent of  $M$ ), so from (2.2),

$$-Nf_b - f_s = 2 \log \Lambda_{\max} , \quad -Nf'_s - f_c = -N \log \Delta + 2 \log \langle \psi|0\rangle . \quad (5.15)$$

We expect these equations to hold in the physical region, where  $0 < u < \lambda/2$  and all the Boltzmann weights are positive. We would like to analytically continue them to  $u > \lambda/2$ .

For the Potts model turned through  $45^\circ$ , with cylindrical boundary conditions, this is not difficult. The eigenvector  $\psi$  is independent of  $u$ , so for finite  $N$  the eigenvalue  $\Lambda_{\max}$  is (after removing the known poles coming from  $e^{K_1}$  and  $e^{K_2}$ ) a polynomial on  $w$ . Here we do not have these properties, but we shall show that if we make some plausible analyticity assumptions, then we can obtain the results (3.26) - (3.31) very simply.

From (5.5) and (5.7), exhibiting the dependence of  $V$  on  $u$ ,

$$V(u)V(\lambda - u) = \xi(u)^N \mathbf{1} . \quad (5.16)$$

Hence if  $\psi$  is the maximal eigenvector of  $V(u)$ , it is also an eigenvector of  $V(\lambda - u)$ . Let  $\Lambda(u)$  and  $\Lambda(\lambda - u)$  be the associated eigenvalues. (For  $0 < u < \lambda/2$  the latter will be the smallest of the eigenvalues.) Then

$$\Lambda(u)^2 \Lambda(\lambda - u)^2 = \xi(u)^N . \quad (5.17)$$

This relation defines  $\Lambda(u)$  is the larger interval  $0 < u < \lambda$ . We *assume* that the resulting function  $\Lambda(u)$  is analytic throughout this extended interval, in particular at the inversion point  $u = \lambda/2$  (apart from a trivial pole of degree  $N$  coming from the double pole of  $\xi(u)$ ).

We also assume that the relations (5.15) can be analytically continued into the extended interval. Then on replacing  $u$  by  $\lambda - u$  in the first relation and using (5.17), we obtain

$$-Nf_b(\lambda - u) - f_s(\lambda - u) = N \log \xi(u) - 2 \log \Lambda_{\max} \quad (5.18a)$$

where  $\Lambda_{\max} = \Lambda(u)$ . Doing the same in the second relation gives

$$-Nf'_s(\lambda - u) - f_c(\lambda - u) = -N \log \Delta(\lambda - u) + 2 \log \langle \psi | 0 \rangle, \quad (5.18b)$$

$\psi$  being unchanged.

Adding (5.18a) to the first of the relations (5.15) (exhibiting the dependence on  $u$ ), we eliminate  $\Lambda_{\max}$ . Then separating the terms linear in  $N$  from those independent of  $N$ , we obtain

$$-f_b(u) - f_b(\lambda - u) = \log \xi(u), \quad -f_s(u) - f_s(\lambda - u) = 0. \quad (5.19a)$$

Subtracting (5.18b) from the second relation (5.15), we eliminate  $\langle \psi | 0 \rangle$  and obtain

$$-f'_s(u) + f'_s(\lambda - u) = \log \frac{\Delta(\lambda - u)}{\Delta(u)}, \quad -f_c(u) + f_c(\lambda - u) = 0. \quad (5.19b)$$

We refer to the four relations (5.19) as the *inversion relations*. There are also four *rotation relations* that can be obtained by noting that replacing  $u$  by  $\lambda/2 - u$  interchanges  $K_1$  with  $K_2$  which is equivalent to rotating the lattice through  $90^\circ$ , so

$$\begin{aligned} f_b(u) &= f_b(\lambda/2 - u) & , & & f_s(u) &= f'_s(\lambda/2 - u) , \\ f'_s(u) &= f_s(\lambda/2 - u) & , & & f_c(u) &= f_c(\lambda/2 - u) . \end{aligned} \quad (5.20)$$

## 5.1 Alternative derivation of the free energies

We shall now show that we can use the above inversion and rotation relations to derive the bulk and surface free energies, and to show that the corner free energy depends only on the parameter  $\lambda$ , but *not* on  $u$ . The method depends on certain analyticity assumptions, so is not rigorous, but it is much simpler than the Bethe ansatz method used above.

### 5.1.1 Assumptions

For finite  $M, N$  the partition function is a finite sum of products of  $e^{K_1}$  and  $e^{K_2}$ , so from (5.2) is a rational function of  $w^2$ . The denominator is a product of at most  $M(N-1)$  powers of  $1 - w^2$ , and of at most  $N(M-1)$  powers of  $1 - q/w^2$ . From (2.2), we therefore expect  $e^{-f_b}$  to have simple poles at  $w^2 = 1$  and  $w^2 = q$ ,  $e^{-f_s}$  to have a simple zero at  $w^2 = 1$ , and  $e^{-f'_s}$  to have a simple zero at  $w^2 = q$ .

Define  $F(u), G(u)$  by

$$e^{-f_b} = e^{K_1+K_2} F(u) \ , \ e^{-f_s(u)} = \frac{(1-w^2) G(u)}{1-q^2/w^2} \ , \quad (5.21)$$

then, consistent with the above remarks and with series expansions, we *assume* that  $\log F(u), \log G(u), f_c(u)$  are single-valued analytic functions of  $w^2$ , not just in the physical regime  $q < w^2 < 1$ , but in an annulus containing  $q \leq |w^2| \leq 1$  in the complex  $w^2$ -plane.

Hence we can write

$$\log F(u) = c_0^{(b)} + \sum_{n=1}^{\infty} [c_n^{(b)} w^{2n} + d_n^{(b)} w^{-2n}] \ , \quad (5.22)$$

$$\log G(u) = c_0^{(s)} + \sum_{n=1}^{\infty} [c_n^{(s)} w^{2n} + d_n^{(s)} w^{-2n}] \ , \quad (5.23)$$

$$f_c(u) = c_0^{(c)} + \sum_{n=1}^{\infty} [c_n^{(c)} w^{2n} + d_n^{(c)} w^{-2n}] \ , \quad (5.24)$$

where the expansions are convergent for  $q \leq |w| \leq 1$ .

We shall show that the relations (5.19), (5.20) then define the coefficients in these expansions, with the sole exception of  $c_0^{(c)}$ . This gives  $f_b, f_s$  and  $f_c$ , and  $f'_s$  is then given by the third of the relations (5.20).

### 5.1.2 Bulk free energy

From (5.19a), (5.20) and (5.22),

$$\begin{aligned} \log F_b(u) + \log F_b(\lambda - u) &= \log \xi(u) - K_1(u) - K_2(u) - K_1(\lambda - u) - K_2(\lambda - u) \\ &= 2 \log(1+q) - \sum_{n=1}^{\infty} \frac{(1-q^n)(w^{2n} + q^{2n}/w^{2n})}{n} \ . \end{aligned} \quad (5.25)$$

Using (5.22) and equating the series term by term, this gives

$$c_0^{(b)} = -\log(1+q) \ , \ c_n^{(b)} + q^{-2n} d_n^{(b)} = (1-q^n)/n \ , \ n > 0 \ . \quad (5.26)$$

Further, the first of the rotation relations (5.20) gives  $\log F_b(u) = \log F_b(\lambda - u)$  and hence  $d_n^{(b)} = q^n c_n^{(b)}$ , so

$$c_n^{(b)} = q^{-n} d_n^{(b)} = \frac{q^n(1-q^n)}{n(1+q^n)} \ , \ n > 0 \ , \quad (5.27)$$

in agreement with our previous result (3.29).

### 5.1.3 Surface free energy

Using (5.20), we can write the first of the relations (5.19b) as

$$f_s(u) - f_s(-u) = \log \frac{\Delta(\lambda/2 - u)}{\Delta(\lambda/2 + u)} = \log \left[ -\frac{\sinh(\lambda + 2u)}{\sinh(\lambda - 2u)} \right] \ . \quad (5.28)$$

Then (5.19a) and (5.23) give  $G(u)G(\lambda - u) = 1$ , and hence from (5.23)

$$c_0^{(s)} = 0 \quad , \quad c_n^{(s)} + q^{-2n} d_n^{(s)} = 0 \quad , \quad n > 0 \quad . \quad (5.29)$$

Also, using (5.20) in the first of the relations (5.28), we obtain

$$f_s(u) - f_s(-u) = \log \frac{\Delta(\lambda/2 - u)}{\Delta(\lambda/2 + u)} = \log \left[ -\frac{(1 - qw^2)}{w^2(1 - q/w^2)} \right] \quad (5.30)$$

which implies

$$-\log G(u) + \log G(-u) = \log \frac{(1 - qw^2)(1 - q^2 w^2)}{(1 - q/w^2)(1 - q^2/w^2)} \quad (5.31)$$

and hence, for  $n > 0$ ,

$$c_n^{(s)} - d_n^{(s)} = \frac{q^n(1 + q^n)}{n} \quad . \quad (5.32)$$

It follows that

$$c_n^{(s)} = \frac{q^n(1 + q^n)}{n(1 + q^{2n})} \quad , \quad d_n^{(s)} = -\frac{q^{3n}(1 + q^n)}{n(1 + q^{2n})} \quad , \quad (5.33)$$

so from (5.23)

$$\log G(u) = \sum_{n=1}^{\infty} \frac{q^n(1 + q^n)(w^{2n} - q^{2n}/w^{2n})}{n(1 + q^{2n})} \quad (5.34)$$

in agreement with our result (3.30).

#### 5.1.4 Corner free energy

Using (5.24), the last of the relations (5.19b), (5.20) give

$$d_n^{(c)} = q^{2n} c_n^{(c)} = q^n c_n^{(c)} \quad , \quad n > 0 \quad . \quad (5.35)$$

Since  $0 < q < 1$ , these equations imply

$$c_n^{(c)} = d_n^{(c)} = 0 \quad , \quad n > 0 \quad . \quad (5.36)$$

Hence we are left with

$$f_c(u) = c_0^{(c)} \quad , \quad (5.37)$$

i.e.  $f_c(u)$  is a constant, independent of  $u$ , and this is in agreement with our conjecture of sub-section 4.2. If Vernier and Jacobsen's conjecture (4.6) is true for the isotropic case, when  $u = \lambda/4$ , then it follows that it must be true for all  $u$ .

## 5.2 Inversion relations for non-solved models

The derivations of the previous sub-section rely on  $\log F(u)$ ,  $\log G(u)$  and  $f_c(u)$  being analytic at the inversion point  $u = \lambda/2, w = q^{1/2}$ , where (5.16) implies that  $V(u)$  is proportional to its inverse. More strongly, they depend on them being analytic in a vertical strip in the complex  $u$ -plane that contains the domain  $0 \leq \text{Re}(u) \leq \lambda/2$ .

There are inversion relations for models that have not been solved, e.g. the square lattice Ising model in a magnetic field, [9]-[11] but the free energies have complicated singularities at the inversion point, and little progress has been made in solving them.



### 5.3 Related work using the reflection relations

Because of our assumptions regarding the analyticity properties of  $\log F(u)$ ,  $\log G(u)$ ,  $f_c(u)$ , the method of this section, while simple, is not rigorous. The reflection Yang-Baxter relations[12]-[15] can be used to obtain functional relations for the transfer matrix eigenvalues, and in a private communication[16] Paul Pearce shows how one can use these to obtain a more rigorous derivation of the inversion relations for the surface free energies.

## 6 Critical behaviour

It is shown in [4, §8.11] that the bulk free energy of the six-vertex model has a singularity at  $\lambda = 0$ , which corresponds to  $Q = 4$  in the Potts model. The singularity is of infinite order, being proportional to  $\exp(-\pi^2/\lambda)$ , i.e.  $\exp[-2\pi^2/(Q-4)^{1/2}]$ . What is the corresponding behaviour of the surface and corner free energies?

To answer this we need the result (4.2) of Owczarek and Baxter[2] for the surface free energy when  $Q < 4$ , which is (replacing  $y$  by  $2y$ )

$$f_s = 2s_\infty = \log \frac{\sin[(\mu+v)/2]}{\sin[(\mu-v)/2]} - \int_{-\infty}^{\infty} \frac{2 \sinh(2vy) \sinh(\pi y - 2\mu y) \cosh(\pi y - \mu y) \cosh(\mu y) dy}{y \sinh(2\pi y) \cosh(2\mu y)} , \quad (6.1)$$

where  $v, \mu$  are given in terms of our  $\lambda, u$  by

$$\mu = -i\lambda , \quad v = -i(\lambda - 2u) \quad (6.2)$$

and the  $Q, x_1, x_2, x$  of ((2.5) and (3.1) above are given by

$$Q^{1/2} = 2 \cos \mu , \quad x_1 = x_2^{-1} = x = \frac{\sin v}{\sin(\mu - v)} . \quad (6.3)$$

In the physical regime(Boltzmann weights positive)  $\mu, v$  are real and  $0 < v < \mu$ . The factor 2 in (6.1) comes from the fact that  $N' = N/2$  in (4.1) of [2]. Also, from (3.15) of [2],  $\sinh[(\pi - 2\mu)y]$  in (4.2) should be  $\sinh[(\pi - 2\mu)y/2]$ .

We can use the identity

$$\sinh(\pi y - 2\mu y) \cosh(\pi y - \mu y) = \sinh(\pi y - 3\mu y) \cosh(\pi y) + \sinh(\mu y) \cosh(2\mu y)$$

to write (6.1) as

$$f_s = \log \frac{\sin(\mu+v)}{\sin(\mu-v)} - \mathcal{P} \int_{-\infty}^{\infty} \frac{\sinh(2vy) \cosh(\mu y) e^{\pi y - 3\mu y}}{y \sinh(\pi y) \cosh(2\mu y)} dy ,$$

$\mathcal{P}$  denoting the principal value integral.

We want to analytically continue this result to  $Q > 4$  so as to compare it with (3.30). We move  $\mu u$  into the lower half plane and can then close the

integration round the upper-half  $y$ -plane. Summing the residues of the poles and using (6.2) gives

$$f_s = \sum_{n=1}^{\infty} \frac{(1 - q^n)(w^{2n} - q^{2n}/w^{2n})}{n(1 + q^{2n})} - 4 \sum_{n \text{ odd}} \frac{[i + (-1)^{(n-1)/2}] \sinh[\pi n(\lambda - 2u)/2\lambda] e^{-\pi^2 n/2\lambda}}{n(1 - e^{-\pi^2 n/2\lambda})} , \quad (6.4)$$

the second sum being over all positive odd integers  $n$ , i.e.  $n = 1, 3, 5, \dots$

Comparing this with (3.27) above, we see that the dominant singularity in  $f_s$  is proportional to  $e^{-\pi^2/2\lambda}$ . This is of infinite order, i.e. all derivatives exist and are continuous. This singularity is proportional to the square root of the dominant singularity in  $f_b$ .

The conjectured expression (4.5) for the corner free energy can be written

$$e^{-f_c} = P(q)^{-1} P(q^2)^{-4} , \quad (6.5)$$

where

$$P(q) = \prod_{k=1}^{\infty} (1 - q^{2k-1}) . \quad (6.6)$$

The function

$$\mathcal{Q}(q) = \prod_{n=1}^{\infty} (1 - q^n) \quad (6.7)$$

occurs in Jacobi elliptic functions and satisfies the “conjugate modulus” relation

$$\mathcal{Q}(q) = \epsilon^{-1/2} \exp \left[ \frac{\pi(\epsilon - \epsilon^{-1})}{12} \right] \mathcal{Q}(q') , \quad (6.8)$$

where if  $q = e^{-2\pi\epsilon}$ , then  $q' = e^{-2\pi/\epsilon}$ . Noting that  $P(q) = \mathcal{Q}(q)/\mathcal{Q}(q^2)$ , it follows that

$$P(q) = \sqrt{2} \exp \left[ -\frac{\pi\epsilon}{12} - \frac{\pi}{24\epsilon} \right] P(q'^{1/2}) , \quad (6.9)$$

and hence that

$$e^{-f_c} = \exp \left( \frac{3\pi\epsilon}{4} + \frac{\pi}{8\epsilon} \right) / \left[ 2^{5/2} P(q'^{1/2}) P(q'^{1/4})^4 \right] \quad (6.10)$$

in agreement with eqn. 81 of [3] (the  $q$  therein is our  $e^{-\pi\epsilon}$ ).

Near the critical point  $Q \rightarrow 4^+$  and  $\epsilon, q' \rightarrow 0^+$ . We see that

$$f_c \sim -\frac{\pi}{8\epsilon} \sim -\frac{\pi^2}{4[2(Q-4)]^{1/2}} , \quad (6.11)$$

so  $f_c$  becomes negatively infinite.

## 7 Summary

In sections 2 and 3 we have adapted previous work[2] on the  $Q$ -state self-dual Potts model on the square lattice from the case when  $Q < 4$  to when  $Q > 4$ . This gives the bulk free energy, which was known[4, eqn. 12.5.6], and also the vertical free energy. We considered the general model, homogeneous but anisotropic. It contains two free parameters, the vertical and horizontal interaction coefficients  $K_1, K_2$ , or equivalently the parameters  $q, w$  defined by (2.5), (3.7), (3.11).

Vernier and Jacobsen[3] had conjectured the bulk, surface and corner free energies for the isotropic case, when  $K_1 = K_2$  and  $w = q^{1/2}$ . We report these conjectures in section 4, and note that our results for the bulk and surface free energies, specialized to this case, agree with their conjectures. We also made series expansions for the more general anisotropic case (taking  $w = q^{1/4}s^{1/2}$ , where  $s$  is a parameter of order unity) and found that the coefficients of the terms in the series were independent of  $s$ . They agreed with Vernier and Jacobsen's conjectures, not just for  $s = 1$ , but for *all*  $s$ .

It is known that the bulk free energy can be easily obtained using the "inversion relation" method[5], [6], [4, §12.5]. In section 5 we show how this can be extended to the surface and corner free energies. Together with the simple rotation relations and appropriate analyticity assumptions, these give an alternative method (simpler than the Bethe ansatz calculation of Owczarek and Baxter[2]) of deriving the surface free energy. They also imply that the corner free energy is a function only of the number of states  $Q$ , in agreement with our series expansions of section 4.

These inversion relation calculations are similar to those for the Ising model.[7]

Finally, in section 6 we discuss the behaviour when  $Q \rightarrow 4^+$  and  $q \rightarrow 1^-$ , which is the critical case of the associated six-vertex model.

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